Gamma-ray Large Area Space Telescope (GLAST)

Large Area Telescope (LAT)

Calorimeter Crystal Optical Test Station Software Requirements

DOCUMENT APPROVAL

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CHANGE HISTORY LOG

Revision	Effective Date	Description of Changes
1	5 March 2001	Initial Release
2	5 July 2001	Revision for version 1.5 of software

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1 PURPOSE

This document specifies the requirements for version 1.0 of the data acquisition and analysis software packages for the GLAST calorimeter crystal testing stations.

2 SCOPE

This document encompasses the whole of the requirements for data acquisition and analysis software for the GLAST calorimeter crystal testing stations.

3 DEFINITIONS

3.1 Acronyms

CAL	LAT calorimeter subsystem
FWHM	Full Width Half Maximum
GLAST	Gamma-ray Large Area Space Telescope
LAT	Large Area Telescope
TBD	To Be Determined
TBR	To Be Resolved

3.2 Definitions

γ	Gamma Ray
μsec, μs	Microsecond, 10^{-6} second
Analysis	A quantitative evaluation of a complete system and /or subsystems by review/analysis of collected data.
cm	centimeter
Demonstration	To prove or show, usually without measurement of instrumentation, that the project/product complies with requirements by observation of results.
eV	Electron Volt
Inspection	To examine visually or use simple physical measurement techniques to verify conformance to specified requirements.
MeV	Million Electron Volts, 10^{6} eV
mm	millimeter
μsec, μs	Microsecond, 10^{-6} second
ph	photons
s, sec	seconds

Simulation	To examine through model analysis or modeling techniques to verify conformance to specified requirements.
Testing	A measurement to prove or show, usually with precision measurements or instrumentation, that the project/product complies with requirements.
Validation	Process used to assure the requirement set is complete and consistent, and that each requirement is achievable.
Verification	Process used to ensure that the selected solutions meet specified requirements and properly integrate with interfacing products.

4 APPLICABLE DOCUMENTS

Documents that are relevant to the development of the crystal testing station software requirements include the following:

4.1 Design Documents

[1] Specification for the Calorimeter CsI Test Bench ADC Control. W. N. Johnson. LAT-SS-nnnnn-D2.

5 DATA ACQUISITION REQUIREMENTS

5.1 Introduction

The calorimeter crystal testing station is used to characterize the scintillation light yield and light attenuation in the CsI(Tl) crystals for GLAST. Scintillation light is measured simultaneously at both ends of a crystal with photomultiplier tubes. A ^{22}Na source is translated along the length of the crystal, and spectra are accumulated event-by-event in the data acquisition system. The electronics for the testing station are described in reference [1].

The data acquisition system software shall be written in LabView and executed under Windows 2000.

The data acquisition system shall accumulate ^{22}Na spectra for a user-definable duration at each of a user-definable set of positions along the length of the crystal under test. The data shall be logged to PC disk either in list mode, where each event is individually recorded, and/or in histogram mode, where events are histogrammed prior to logging. The data shall be analyzed by the software described in section 6.

5.2 Interface

The user shall interact with the acquisition software through a GUI. The user shall control the data acquisition through a single window that enforces certain standards for acquisition (Section 5.3.1). There shall be a status display during acquisition (Section 5.5). On successful completion of the crystal scan and logging of data to disk, the software shall notify the user with some suitably happy message.

5.3 Inputs

5.3.1 Control inputs

The user interface shall provide for a number of input parameters at run time to define or describe the data acquisition. The parameters are specified below. Some are required, while others are optional with a default value. In typical use, the operator will specify the Crystal ID number, his or her name, the ambient temperature and humidity, and leave all other entries at their default settings.

The default settings shall be specified in an ASCII Setup file. The Setup file shall have filename `acquire.ini`. It shall have the format given in Table 1.

Table 1: Format of `acquire.ini`, the Setup file for the acquisition software

```
Operator = Name
Operators Location = Location
Data directory = d:\data
Positions = [28,56,84,112,140,168,196,224,252,280,308]
Accumulation time = 500
Comment = None.
Temperature = 0.0
Humidity = 0
High voltage 0 = -1000
High voltage 1 = -1000
ADC gain = 1024
ADC range = 1024
Shaper 0 Fine Gain = 4.5
Shaper 0 Coarse Gain = 40
Shaper 1 Fine Gain = 4.5
Shaper 1 Coarse Gain = 40
Data mode = 3
Distance from Home to 0 (mm) = 64
Home search granularity (steps) = 8
DIO-32HS Buffer Size (scans) = 128000
High Volt delay time (ms) = 500
Coincidence time (2|4|8|16) usec = 2
Motor controller port (serial) = 1
```

5.3.1.1 Crystal ID

A 64-character string specifying the identification number of the crystal to be scanned. This is a required parameter. A typical crystal ID might have the form `<Vendor>-<Lot number>-<Item number>`, but the software shall not enforce any particular standard form (TBR). The acquisition software shall substitute underscores for any periods or blank spaces in the Crystal ID number, and it shall terminate the ID number with an underscore, "_". *Note: we will likely specify a standard form for Crystal ID at a future date.*

5.3.1.2 Operator

A 64-character string specifying the operator's name. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be "Name".

5.3.1.3 Operator's Location

A 64-character string specifying the geographic location of the operator. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be "Location".

5.3.1.4 Data Directory

A string specifying the directory into which data are written. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be TBD.

5.3.1.5 Version

A 2-character string indexing the number of times the specified crystal has been scanned. This is a required parameter, with special behavior: the acquisition software shall query the Data Directory to find the most current scan of this Crystal ID and prompt the user with the appropriate Version index. The initial Version index shall be 'a', and it shall increase alphabetically from 'a' to 'z', then 'aa' to 'zz'. The Version index shall be tied to prior uses of Crystal ID, rather than Crystal ID and Position; thus if data files from a given Crystal ID are present at the start of a scan, the acquisition software shall use the subsequent Version index, regardless of the prior and chosen current Positions. The Version index for list mode and histogram mode files shall not be independent, e.g. if a '*b.lis' exists, the next version index shall be 'c', regardless of whether the accumulation is list mode or histogram mode.

5.3.1.6 Positions

A numerical floating-point array listing the scan positions to be analyzed in units of millimeters from the home position. This is a required parameter with default read from the Setup file. The nominal set of positions in the initial Setup file shall be [28,56,84,112,140,168,196,224,252,280,308], i.e. 11 positions uniformly spaced by 28 mm.

There shall be a "Reset Current Positions" button that, if selected, clears all entries in the Positions array.

There shall be a "Reload Default Positions" button that, if selected, reloads the Positions array from the Setup file.

There shall be a "Use calibration fiducial only" check box that, if selected, overrides any locations previously entered in the Positions field, sets Positions to the single value 168 (i.e. the nominal center of the crystal), and displays single value in the Positions field. This button is intended to be used when the operator wishes to calibrate the response of the data acquisition system with a standard, calibrated crystal.

5.3.1.7 Accumulation Time

An integer value specifying the time in seconds over which data shall be accumulated at each position. This is a required parameter with default set by the Setup file. The nominal value in the Setup file shall be 500 seconds.

5.3.1.8 Comment

A string containing up to 256 characters describing any special situation relevant to the data being accumulated. This is an optional parameter, with default set by the Setup file. The nominal value in the Setup file shall be "None".

5.3.1.9 Temperature

A floating point number containing the ambient temperature (in degrees C) at the start of data acquisition. This is a required parameter with default set by the Setup file. The nominal value in the Setup file shall be 0.0; this value shall also be used to indicate "No measurement". The temperature measurement shall be made manually with external instrumentation.

5.3.1.10 Humidity

An integer number indicating the relative humidity (in %) at the start of data acquisition. This is a required parameter with default set by the Setup file. The nominal value in the Setup file shall be 0; this value shall also be used to indicate "No measurement". The humidity measurement shall be made manually with external instrumentation.

5.3.1.11 High Voltage 0 and 1 Controls

Two integer values containing high voltage settings (in volts) for the photomultiplier tubes. These are required parameters with default values specified in the Setup file. The nominal value in the Setup file shall be –1000V. High voltage settings shall be constrained to be within 0V and –1500V. A setting more negative than –1500V shall be forced to –1500V. High voltage settings shall always be negative. The high voltage settings shall be converted to HV DAC units as specified in the hardware description (Ref. [1]). The setup GUI window shall indicate through highlight or color that the HV values are indeed controls for the HV power supplies, rather than merely indicators of the hardware status.

5.3.1.12 ADC Gain

An integer value indicating the number of bins into which the full-scale input voltage (10V) will be divided, as indicated by the rotary switch on the front panel of the ADCs (assumed to be Canberra 8071). Both ADCs shall be set to the same gain. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 1024.

5.3.1.13 ADC Range

An integer value indicating the number of bins in the ADC digitization, as indicated by the rotary switch on the front panel of the ADCs (assumed to be Canberra 8701). Both ADCs shall be set to the same range. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 1024.

5.3.1.14 Shaper 0 and 1 Coarse Gain

An integer value indicating the number of bins into which the full-scale input voltage (10V) will be divided, as indicated by the rotary switch on the front panel of the shaping amp (assumed to be an Ortec 855 dual spec amp). This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 4096.

5.3.1.15 Shaper 0 and 1 Fine Gain

Two floating-point values containing the Fine Gain settings of the shaping amplifiers, as indicated on the rotary, 10-turn potentiometer on the front panel of the amp (assumed to be an Ortec 855 dual spec amp). These are required parameters with default value specified in the Setup file. Each full turn of the pot shall be noted with the units digit, and fractional turns with the decimal values. The nominal value in the Setup file shall be 4.50.

5.3.1.16 Data Mode

A pull-down menu specifying one of four modes in which data are written to disk: "List mode with time stamps", "List mode without time stamps", "Histogram mode", or a combined mode in which "List mode without time stamps" and "Histogram mode" data are written in separate files. This is a required parameter, with default set to histogram mode. In both list modes, the data are logged to disk event by event, with each event generating an optional time stamp and two digitized pulse heights (Section 5.6.2.2). In the output header record (Section 5.6.2.1), the modes shall be referred to by number: 0 = list mode with time stamps; 1 = list mode without time stamps; 2 = histogram mode; and 3 = simultaneous list mode without time stamps and histogram mode.

5.3.1.17 Distance from Home to Zero

An integer value indicating the distance (in mm) measured between the axis of the collimated ^{22}Na beam when the source is at the starting limit switch, i.e. "Home", and when the source is aligned with the start of the crystal. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 64, which is the proper value for the first Crystal Optical Testing Station built at NRL. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.3.1.18 Home Search Granularity

An integer value indicating the granularity (in units of motor steps) of the search for the Home position. To find Home, the motor shall drive to the limit switch and record the step location, then back off a number of steps equal to Home Initial Guesses to release the limit switch, then drive toward the limit switch the same distance. If the limit switch is closed after the return stepping, then the switch shall be deemed to be found. If not, the search process shall begin again. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 8. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.3.1.19 DIO-32HS Buffer Size

An integer value indicating the number of spectra that can be stored in the I/O interface card. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 128000. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.3.1.20 High Voltage Delay Time

An integer value indicating the delay between (in ms). This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 500. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.3.1.21 Coincidence Time

An integer value indicating the duration of the coincidence window (in μs) between the two ADCs. This is a required parameter with default value specified in the Setup file. Acceptable values shall be limited to 2, 4, 8, and 16. The nominal value in the Setup file shall be 2. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.3.1.22 Motor Controller Port

An integer value indicating the serial port ID to which the motor controller board is attached. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be 1. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.3.1.23 Steps Per mm

An integer value indicating the number of motor drive steps per mm of distance traveled. This is a required parameter with default value specified in the Setup file. The nominal value in the Setup file shall be TBD. This value shall not be accessible through the GUI; rather it shall be present only the Setup file.

5.4 Run Controls

5.4.1 Run

The shall be a "Run" button to begin a scan of a crystal. When this button is selected, the source shall translate to its home position, then to the first position (Section 5.3.1.6), and a spectrum shall be accumulated for the specified length of time (Section 5.3.1.7). When an accumulation is completed, the source shall translate to the next position in the list, and a new accumulation shall be started. When the list of positions is exhausted, the user shall be notificed that the scan is complete, and the source shall translate to its home position. If a scan is in progress, this button shall be disabled.

5.4.2 Stop this accumulation

There shall be a "Stop this accumulation" button to terminate the current accumulation of data. Adjacent to the button, there shall be explanatory text describing the function of this button. There shall be a pop-up dialog box to confirm the decision to stop this accumulation. If this button is selected and confirmed, the current data acquisition shall stop, the source shall translate to the next position, and data acquisition shall begin again. The user shall be notified that the current accumulation has been terminated and that the next accumulation will begin.

5.4.3 Kill this scan

There shall be a "Kill this scan" button to terminate the entire scan of the current crystal. Adjacent to the button, there shall be explanatory text describing the function of this button. There shall be a pop-up dialog box to confirm the decision to kill this scan. If this button is selected and confirmed, the current data acquisition shall stop, the source shall translate to its home position, and no further acquisitions shall occur. The user shall be notified that the scan has been terminated and that the source is going home.

5.5 Runtime display

The runtime display shall consist of three histograms and a status window. The histograms shall contain the spectra from each PMT and from the event-by-event average of both PMTs. The histograms and status information (see below) shall be updated every 2 seconds, or as defined by the user in the runtime display.

During data acquisition, the status window shall display the current output data filename, the data output mode (Section 5.3.1.14), the range of both ADCs (i.e. the number N of bins in histogram mode, or the number of ADC bins in list mode), the number of seconds into the accumulation (updated every TBD seconds) and the total number of seconds to be accumulated (Section 5.3.1.7), the number of events logged (updated every TBD events), the location of the translation stage (in mm from the Home position), and a red/green "LED" to indicate the current status of the accumulation (red = stopped, green = acquiring data).

The run time display window shall have panic buttons that duplicate the "Stop this accumulation" and "Kill this scan" functions from the control window.

5.6 Outputs

The accumulated spectra shall be written to PC disk. In list mode, the data are written event by event in binary as two two-byte integers. In histogram mode, the data are accumulated into histograms, one of each ADC and one for the average of the two ADCs, and written as three consecutive N-bin histograms.

5.6.1 File name

The names of output data files shall be computed automatically. They shall the form `Crystal ID + Position(i) + Version + Extension`, where `Extension` is '.lis' for both list modes and '.his' for histogram mode, and the other variables are defined above. The floating-point position shall be truncated to the nearest integer millimeter. The data acquisition software shall display the output file name for the current acquisition in the Run tme display (Section 5.5). The data analysis software shall use the same file naming convention.

5.6.2 File formats

The data files shall have a header record followed by data records. The data shall be written in binary.

5.6.2.1 Header record

The data file shall begin with a header record in the format shown in Table 2. The header format is independent of the data mode. Fields are as described in the cross-referenced sections, or as described below.

The date and time at the start of data acquisition shall be computed and logged to the header record in integer YYYYMMDD and HHMMSS format. The hardware control/status register and the mask register shall be logged to the header record.

Table 2: Format of output header record

Field	Type	Reference
File name	128-char string	Section 5.6.1
Software version	8-char string	Version number of acquisition software
Start date	4-byte integer	YYYYMMDD of date at start of acquisition
Start time	4-byte integer	HHMMSS of day at start of acquisition
Operator	64-char string	"Collected by " + Section 5.3.1.2
Operator's location	64-char string	Section 5.3.1.3
Crystal ID	64-char string	Section 5.3.1.1
Version	2-char string	Section 5.3.1.5
Position	4-byte float	Section 5.3.1.6, current position only
Accum time	2-byte integer	Section 5.3.1.7
Live time	4-byte integer	See hardware description, ref. [1]
Comment	256-char string	Section 5.3.1.8
Control/status register	2 byte unsigned integer	See hardware description, ref. [1]
Mask register	2 byte unsigned integer	See hardware description, ref. [1]
Temperature	4-byte float	Section 5.3.1.9
Humidity	2-byte integer	Section 5.3.1.10
High voltage DAC 0	2-byte integer	Section 5.3.1.11
High voltage DAC 1	2-byte integer	Section 5.3.1.11
Fine gain, shaper 0	4-byte float	Section 5.3.1.15
Coarse gain, shaper 0	2-byte integer	Section 5.3.1.14
Fine gain, shaper 1	4-byte float	Section 5.3.1.15
Coarse gain, shaper 1	2-byte integer	Section 5.3.1.14
ADC gain	2-byte integer	Section 5.3.1.12
ADC range	2-byte integer	Section 5.3.1.13
Data mode	2-byte integer	Section 5.3.1.14

5.6.2.2 Data record

In list mode with time stamps, the data shall be written one event at a time as a time-stamp quad-word, followed by the two ADC values stuffed into two 16-bit unsigned integers. The ADC values from the two channels shall be written in readout order. The format is shown in Figure 1.

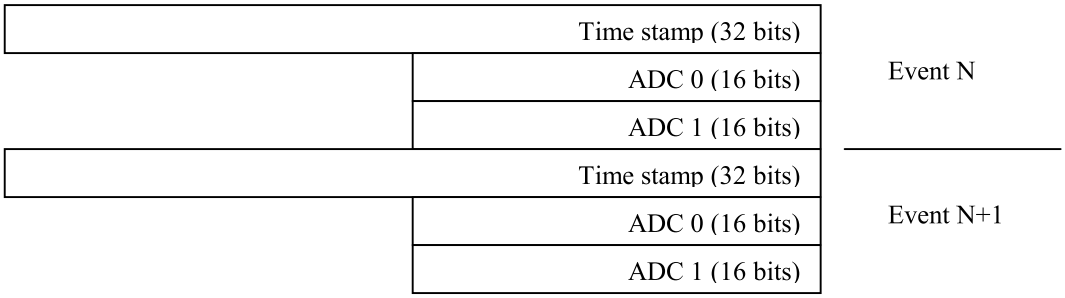


Figure 1: Format of data in list mode with time stamps

In list mode without time stamps, the data shall be written one event at a time as the two ADC values stuffed into two 16-bit unsigned integers. The ADC values from the two channels shall be written in readout order. The format is shown in Figure 2.

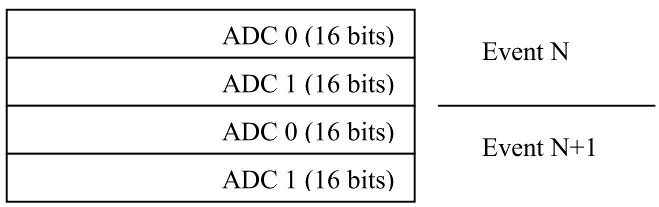


Figure 2: Format of data in list mode without time stamps

In histogram mode, the data shall be written as three consecutive N-bin histograms, one for each ADC and one for the average of the two ADCs, in hardware readout order. Each bin shall be represented by a 2-byte integer. The format is shown in Figure 3.

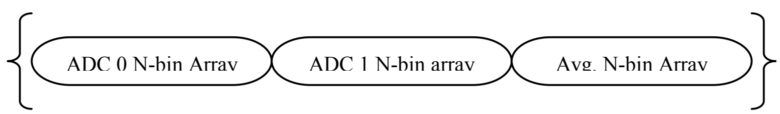


Figure 3: Format of data in histogram mode

6 DATA ANALYSIS REQUIREMENTS

6.1 Introduction

The data analysis system shall be written in LabView.

The data analysis system shall fit the 511 keV line from β^+ decays of ^{22}Na. It shall autonomously find the region around the 511 keV peak and fit the spectrum with a model consisting of a gaussian line and exponential + constant background, as described below.

6.2 Interface

The user shall interact with the analysis software through a GUI. The user shall control the data analysis through a single window that enforces certain analysis standards (Section 6.3). By default, the analysis shall pause between each successful spectral fit to allow the user to confirm the quality of the fit. The analysis software shall create a number of diagnostic plots and tables to document the results of its spectral modeling (Section 6.7). On successful completion of the analysis of the full crystal scan dataset and logging of fits to disk, the software shall notify the user with some suitably happy message.

6.3 Inputs

6.3.1 Data inputs

The analysis system shall read both list-mode and histogram-mode data from the crystal testing station data acquisition system. The list-mode and histogram-mode file formats are given in Section 5.6.2. The input data files shall have names of the form `Crystal ID + Position(i) + Version + Extension`, where `Extension` is '.lis' for both list modes and '.his' for histogram mode, and the other variables are defined below. The data acquisition software shall use the same file naming convention.

If the data are written in list mode, they must be histogrammed prior to fitting. The number of bins in the histogram is given by the ADC Range value from the header record (Section 5.3.1.13). In addition, the analysis software search for the maximum ADC value in the data stream and verify that it does not exceed the ADC Range header value. If maximum value exceeds the ADC Range, the software shall find the smallest number 2^n greater than the maximum value, rewrite the data file with the proper ADC range, and warn the user that the ADC Range header value was incorrect and has been modified. The analysis software shall histogram the two ADC channels independently (with number of bins equal to ADC Range), and it shall pass these histograms on to the searching and fitting routines.

6.3.2 Control inputs

The user interface shall provide for a number of input parameters at run time to define or describe the analysis technique. The parameters are specified below. Some are required, and others are optional with a default value.

The default settings shall be specified in an ASCII Setup file that is read by the analysis software. The Setup file shall have filename `analysis.ini`. It shall have the format given in Table 3.

Table 3: Format of `analysis.ini`, the Setup file for the analysis software

```
Operator = Name
Data directory = d:\xots\data
Output directory = d:\xots\fits
Comment = None
Confirm fits before proceeding = Yes
Save plots of fits = Yes
Smoothing window (bins) = 30
Threshold (bin) = 50
Start of fit range (multiplier) = 0.6
Lower bound of start of fit range (bin) = 100
End of fit range (multiplier) = 1.6
Lower bound of end of fit range (bin) = 300
Upper bound of end of fit range (bin) = 900
Number of bins to avg for const bkg = 10
Lower bound of parameter A = 100
Upper bound of parameter A = 1000000
Lower bound of X0 (Start of fit range + X bins) = 10
Upper bound of X0 (End of fit range – X bins) = 10
Lower bound of sigma = 10
Upper bound of sigma = 200
Lower bound of B = 10
Upper bound of B = 1000000
Lower bound of tau = 1
Upper bound of tau = 1000
Lower bound of C = 0
Upper bound of C = 1000000
Min acceptable mean of avg centroid (bins) = 1
Max acceptable mean of avg centroid (bins) = 4095
Max acceptable mean of avg FWHM (%) = 15
Max acceptable peak to peak dev (%) = 10
Min acceptable taper, far/near (%) = 50
Max acceptable taper, far/near (%) = 70
```

6.3.2.1 Crystal ID

A 64-character string specifying the identification number of the crystal to be scanned. This is a required parameter. The Crystal ID shall have the same format as that in Section 5.3.1.1. The analysis software shall substitute underscores for any periods or blank spaces in the crystal ID number, and it shall terminate the ID number with an underscore, "_". The crystal ID shall resolve to a value identical to that in Section 5.3.1.1.

6.3.2.2 Operator

A 64-character string specifying the operator's name. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be "Name".

6.3.2.3 Operator's Location

A 64-character string specifying the operator's geographic location. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be "Location".

6.3.2.4 Data Directory

A string specifying the directory in which the data can be found. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be "d:\xots\data".

6.3.2.5 Output Directory

A string specifying the directory to which the various output files (Section 6.7) shall be written. This is a required parameter with default set to its previous contents. The nominal value in the Setup file shall be "d:\xots\fits".

6.3.2.6 Version

A two-character string indexing the number of times the specified crystal has been scanned. This is a required parameter, with special behavior: the analysis software shall query the data directory to find the most current scan of this crystal ID and prompt the user with the corresponding Version index. The initial Version index shall be 'a', and it shall increase alphabetically from 'a' to 'z', then 'aa' to 'zz'. The Version index for the analysis shall be identical to the Version index of the data file.

6.3.2.7 Positions

A numerical floating-point array listing the scan positions to be analyzed. Units are distance from home position in millimeters. This is a required parameter, with special behavior: the analysis software shall query the data directory for files at all positions for the current Version for this crystal ID and prompt the user with the corresponding list of positions. The user shall have the option of editing this list to restrict the fitting to a subset of positions.

6.3.2.8 Comment

A string containing up to 256 characters describing any special situation relevant to the data being analyzed. This is an optional parameter, with default specified in the Setup file. The nominal value in the Setup file shall be 'None.'

6.3.2.9 Confirm fits before proceeding?

A pair of radio buttons indicating 'Yes' or 'No.' This is a required parameter with default specified in the Setup file. The nominal value in the Setup file shall be 'Yes.' If 'Yes', the analysis shall pause between spectral fits until the user acknowledges a 'Ready to proceed?' question. The confirmation window shall not interfere with the fit display (see Section 6.7.2). If 'No', the analysis shall pause for 5 seconds between fits, proceeding without confirmation from the user.

6.3.2.10 Create GIF of spectral fits?

A pair of radio buttons indicating 'Yes' or 'No.' This is a required parameter with default specified in the Setup file. The nominal value in the Setup file shall be 'Yes.' If 'Yes', the graphical display (see Section 6.7.2) of each fit shall be logged to disk in GIF format. The plot file name shall be `Crystal ID + Position(i) + Version + ".gif"`.

6.3.2.11 Search constraints

The analysis software searches the spectrum for the likely location of the 511 keV line, and makes a set of initial guesses for the fit parameters, as described below. The contraints of the search for the 511 keV line and the initial guesses for the fit shall be adjustable from a pop-up window. The search constraints are defined in section 6.5.1, and the default values are given in Table 4.

Table 4: Default values for search constraints

Search Constraint	Default value
Smoothing window	50 bins
Threshold bin	50
Start of fit range, multiplier	0.6
Lower bound of start of fit range	100 bins
End of fit range, multiplier	1.6
Lower bound of end of fit range	300 bins
Upper bound of end of fit range	2000 bins
Number of bins averaged to give constant bkg level	10 bins

6.3.2.12 Parameter bounds

The constraints for the model parameters shall have default values specified in Table 5. The user shall have the option of overriding those values in a pop-up window. For clarity for the user, the pop-up window shall display the functional form of the fit model, as shown in Section 6.4.

6.4 Fit model

The analysis software shall fit the 511 keV line with a model consisting of a gaussian line and exponential + constant background.

$$f(x) = \frac{A}{\sqrt{2\pi\sigma^2}} \exp[-(x-x_0)^2/2\sigma^2] + B\exp[-(x-x_B)/\tau] + C$$

The free parameters of the model are the gaussian integral A, centroid x_0, and rms σ, the exponential amplitude B at x_B, and e-folding length τ, and the constant level C. To ensure that the gaussian integral A is properly normalized, the model function shall be integrated over the bin width. The parameters shall be stored in the fit data structure (see Section 6.6 and Table 6) in the order A, x_0, σ, B, x_B, τ, C. The exponential offset x_B is fixed by the data set (and is therefore not a free parameter of the fit), and all free parameters are bounded.

6.4.1 Partial derivatives of model function

For certain models and parameter estimation algorithms, the results are more robust if the analytic partial derivatives of the model function with respect to its parameters are explicitly used. Furthermore, by fixing the partial derivative of the exponential offset x_B identically to zero, one can fix that parameter at its initial value, i.e. not allow it to be a free parameter. The analysis software shall use the analytic partial derivatives, and it shall force the derivative of the exponential offset to be identically zero. The partial derivates are listed below.

$$\frac{\partial f}{\partial A} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-(x-x_0)^2/2\sigma^2]$$

$$\frac{\partial f}{\partial x_0} = \frac{A}{\sqrt{2\pi\sigma^2}} \exp[-(x-x_0)^2/2\sigma^2] \frac{(x-x_0)}{\sigma^2}$$

$$\frac{\partial f}{\partial \sigma} = \frac{A}{\sqrt{2\pi\sigma^2}} \exp[-(x-x_0)^2/2\sigma^2] \left(\frac{(x-x_0)^2}{\sigma^3} - \frac{1}{\sigma} \right)$$

$$\frac{\partial f}{\partial B} = \exp[-(x - x_B)/\tau]$$

$$\frac{\partial f}{\partial x_B} = B\exp[-(x - x_B)/\tau]\left(\frac{1}{\tau}\right) \equiv 0$$

$$\frac{\partial f}{\partial \tau} = B\exp[-(x - x_B)/\tau]\,\frac{(x - x_B)}{\tau^2}$$

$$\frac{\partial f}{\partial C} = 1$$

6.5 Fit process

The best-fit model parameters shall be derived using a Levenberg-Marquardt non-linear least-squares chi-squared minimization procedure. The data to be fit shall be the spectra of the individual data acquisition channels, and the uncertainty in each bin shall be the square root of the number of counts in the bin. The fitting process shall be robust and shall fail gracefully, reporting errors to the user and continuing to the next data set.

The fitting process is sensitive to the region over which the fit is expected to model the data. The fitting range shall be selected according the procedure defined in Section 6.5.1.

The fit parameters shall be bounded according to the procedure defined in Section 6.5.2.

6.5.1 Selection of fitting range and initial guesses for parameters

The fitting range and initial guess for the free parameters shall be derived by the following process.

1. Smooth the data with a 50-bin running average. The smoothing window shall be user-adjustable.
2. Calculate the first derivative of the smoothed data set, bin by bin, as *deriv(i) = smooth(i+1) – smooth(i)*.
3. The left half-maximum (*LHM*) is the first maximum in the derivative above a threshold bin. The threshold bin shall be 50, by default. The threshold bin shall be user-adjustable.
4. The right half-maximum (*RHM*) is the first minimum in the derivative greater than the left half-maximum.
5. The initial guess for the gaussian rms shall be $\sigma = (RHM - LHM) / 2.35$.
6. The initial guess for the gaussian centroid shall be $x_0 = (RHM + LHM) / 2$.
7. Select the fitting range based on the guess at the centroid location. The start of the fit range shall be $0.6x_0$, but it shall not be less than 100 bins. The end of the fit range shall be $1.6x_0$ but it shall not be less than 300 bins or greater than 2000 bins. The multiplier for the start of the fit range and the minimum value of the start of the fit range shall be user-adjustable. The multiplier for the end of the fit range and the minimum and maximum values for the end of the fit range shall be user-adjustable.
8. The initial guess for the constant C shall be the mean value of the last 10 bins in the fit range.
9. The initial guess for the exponential amplitude B shall be the value of the first bin in the fit range minus the constant C.
10. The offset for the exponential x_B shall be defined to be the start of the fit range. It is fixed, not a free parameter.
11. The initial guess for the e-folding length τ shall be given by τ = *(number of bins in fit range) / $\log_e$(value at last bin in fit range / value at first bin in fit range)*.
12. The initial guess for the gaussian amplitude A shall be $A = (RHM - LHM) \times (\text{value at } x_0 - C)$.

6.5.2 Parameter bounds

The fit parameters shall be constrained by bounds given in Table 5. The parameter bounds shall be adjustable by the user.

Table 5: Bounds on fit parameter

Parameter	Lower bound	Upper bound
A	10^2	10^6
x_0	Start of fit range + 10 bins	End of fit range – 10 bins
σ	10 bins	200 bins
B	10	10^6
τ	1	10^3
C	0	10^6

6.6 Fit data structure

Results of the fits shall be stored in an array of data structures defined in Table 6. ‘LHS’ is the ‘left-hand side’, and ‘RHS’ is the ‘right-hand side.’ The array of structures shall be written to disk (Section 6.7.1) at completion of the fits.

Table 6: Data structure for best-fit model

Field	Type	Reference
Data file name	128-char string	Name of input data file
Software version	8-char string	Version of fitting software
Acquisition date	4-byte integer	Copied from data file header
Acquisition time	4-byte integer	Copied from data file header
Acquisition operator	64-char string	Copied from data file header
Acquisition temperature	4-byte float	Copied from data file header
Acquisition humidity	2-byte integer	Copied from data file header
Acquisition ADC gain	2-byte integer	Copied from data file header
Acquisition ADC range	2-byte integer	Copied from data file header
Fit date	4-byte integer	YYYYMMDD of date of LHS fit
Fit time	4-byte integer	HHMMSS time of day of LHS fit
Operator	64-char string	"Analyzed by " + Section 6.3.2.2
Operator's location	64-char string	Section 6.3.2.3
Crystal ID	64-char string	Section 6.3.2.1
Comment	256-char string	Section 6.3.2.8
Position	4-byte float	Section 6.3.2.7, current position only
LHS spectrum	4-byte integer array, N elements	Spectrum read from data file, N = ADC range
LHS fit parameters	4-byte float array, 7 elements	Best-fit model parameters
LHS fit parameter errors	4-byte float array, 7 elements	68%-confidence uncertainties in model parameters
LHS chi-squared	4-byte float	Chi-squared of best fit
RHS spectrum	4-byte integer array, N elements	Spectrum read from data file, N = ADC range
RHS fit parameters	4-byte float array, 7 elements	Best-fit model parameters
RHS fit parameter errors	4-byte float array, 7 elements	68%-confidence uncertainties in model parameters
RHS chi-squared	4-byte float	Chi-squared of best fit
Average spectrum	4-byte integer array, N elements	Spectrum read from data file, N = ADC range
Avg fit parameters	4-byte float array, 7 elements	Best-fit model parameters
Avg fit parameter errors	4-byte float array, 7 elements	68%-confidence uncertainties in model parameters
Avg chi-squared	4-byte float	Chi-squared of best fit

6.7 Outputs

The analysis software shall produce a number of output figures and tables to document the performance of the crystal under study. The various outputs that are written to disk shall be written to the directory specified at run time (Section 6.3.2.5).

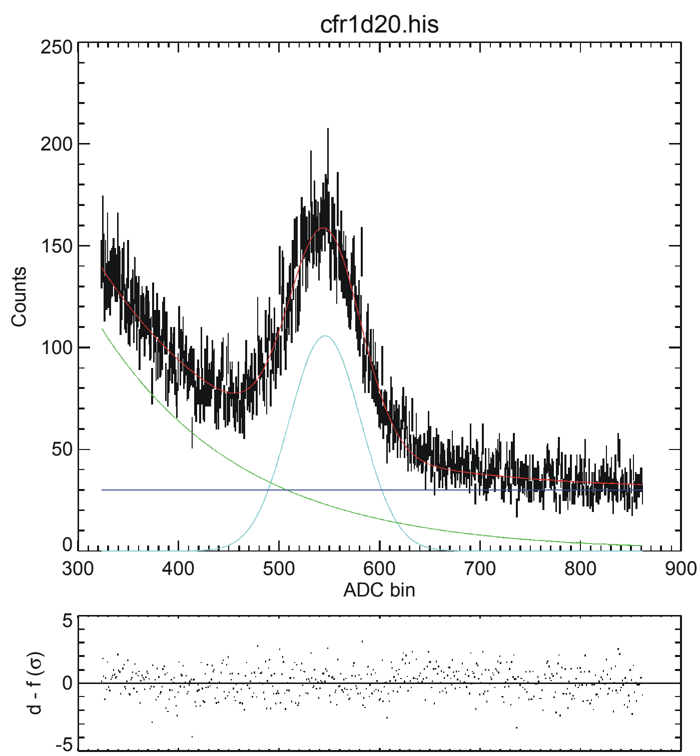
6.7.1 Fit data structure

At the completion of all of the spectral fitting, the analysis software shall write the array of fit data structures (Section 6.6) to disk. The structure shall be written in binary to file `Crystal ID + Version + '_fit.str'`.

6.7.2 Graphical display of best fit

The analysis software shall produce a graphical display for each spectrum fit of the spectral data, the best-fit model, and the components of the model similar to that shown in Figure 4. The plot is labeled with the input data filename. The upper panel shows the spectral data as counts per bin and uncertainties equal to the square root of the number of counts. The model and its components are displayed in complementary colors. The middle panel shows the deviation from the best-fit model in units of statistical uncertainty [i.e. *(<data at bin i> – <model at bin i>) / <sqrt(data at bin i)>*]. The bottom panel shows the reduced chi-squared, the best-fit model parameters, and their uncertainties (68%).

The graphical display shall be drawn to the screen. If the 'Confirm fits before proceeding?" button is checked, the software shall wait until the user acknowledges a 'Ready to proceed?' question. The confirmation window shall not interfere with the fit display. If the 'Confirm fits' box is not checked, the analysis shall pause for 5 seconds between fits, proceeding without confirmation from the user. If the "Create hardcopy of fits?" box is checked, the display shall be logged to disk in JPEG format. The display file shall be named `Crystal ID + Position(i) + Version + Extension`, where `Extension` is `'_LHS.jpg'` or `'_RHS.jpg'` for the left-hand side or right-hand side, respectively.




```
2000 Dec 18 10:06
   ChiSqr/Dof:  1.082  NDof =   533  (Prob =  0.092915)
   Channel Range:    323. -  862. bins
   Integrating Gaussian
No        P             dP          Pmin-P        Pmax-P    Cnstr  Par_Name
 1    9424.8125     230.5159                                BOUND  Gauss Integral
 2      83.7358       1.7715                                BOUND  FWHM
 3     545.6487       0.6580                                BOUND  Centroid
   Exponential Function
 1     109.6250       1.9082                                BOUND  Amplitude
 2     142.2932       7.7667                                FREE   E-folding Length
 3     323.0000                                             FIXED  Normalizing Chan
   Constant Function
 1      30.0223       0.9741                                SIGN+  Constant
```

Figure 4: Example of graphical display of best fit of 511 keV line from ^{22}Na in Crystal Testing Station.

6.7.3 Graphical display of centroid as a function of position

The analysis software shall produce a single graphical display of the best-fit centroids for left and right ends as a function of position (i.e. distance from Home), similar to that shown in Figure 5. This centroid as a function of position shows the "light-tapering function." The light-tapering functions from the two ends shall be shown with distinct plot symbols, and each point shall be drawn with the rms of the centroid as a vertical error bar. The plot shall be drawn to the user's screen and logged to a file in JPEG format with filename `Crystal ID + Version + '_taper.jpg'`.

6.7.4 Table of pulse heights

The analysis software shall produce an ASCII table of the best-fit centroid and rms measured at each end for each test position. The table shall also contain several summary lines as indicated in the following paragraphs and in Table 7. This table shall be written to the user's screen and shall be logged to a file with filename `Crystal ID + Version + '.txt'`. The fields of the table logged to file shall be tab-separated to allow reading by a commercial spreadsheet program. An example is shown in Table 7.

The "Mean of avg centroid (bins)" is defined to be the mean of the best-fit centroids of the average-of-two-ends. The "Mean of avg FWHM (%)" is defined to be the mean of the best-fit rms of the average-of-two-ends converted to the FWHM as follows: Mean of avg FWHM (%) = 235 × {Σ[avg rms (bins)] / (number of positions)} / Mean of avg centroid (bins). The "peak to peak dev[iation] of average (%)" is defined to be (largest of avg centroids) – (smallest of avg centroids) / (Mean of avg centroid), in percent. The "LHS taper, far/near (%)" is defined to be ratio of the centroid at the greatest position to the centroid at the smallest position, in percent. In constrast, the "RHS taper, far/near (%)" is defined to be ratio of the centroid at the smallest position to the centroid at the greatest position, in percent. The LHS and RHS "FWHM (%)" are defined to be 235 × rms (bins) / centroid (bins).

The analysis software shall test summary quantities against limits defined in the Setup file `analysis.ini` and display either "pass" or "FAIL" in a third column following the summary quantities. The "Mean of avg centroid" shall "pass" if it is greater than or equal to the minimum acceptable value and less than or equal to the maximum acceptable value listed in the Setup file; otherwise, it shall "FAIL". The "Mean of avg FWHM" shall "pass" if it is less than or equal to the maximum acceptable value in the Setup file; otherwise it shall "FAIL". The "Peak to peak deviation of

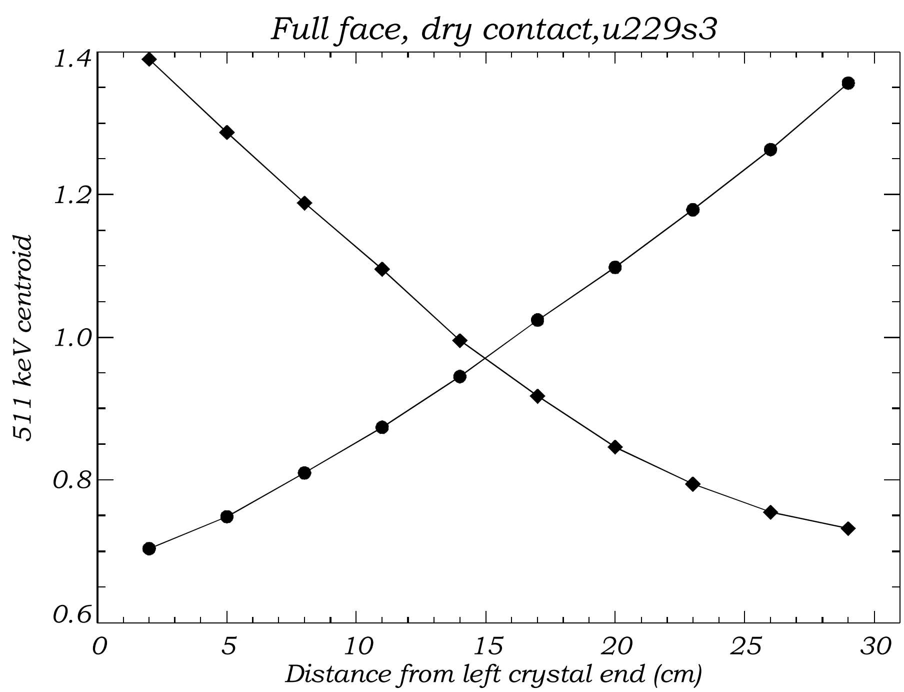


Figure 5: Example graphical display of light tapering function

avg" shall "pass" if it is less than or equal to the maximum acceptable value in the Setup file; otherwise it shall "FAIL". The LHS and RHS "taper, far/near" shall "pass" if it is greater than or equal to the minimum acceptable value and less than or equal to the maximum acceptable value listed in the Setup file; otherwise, it shall "FAIL". The default values for the limits are given in Table 3.

Table 7: Example ASCII table dump of best-fit centroids, rms, and summary values. Fields are tab separated. Intermediate positions have been elided.

Mean of avg centroid (bins)			334.2	Pass					
Mean of avg FWHM (%)			12.9	Pass					
Peak to peak dev of avg (%)			3.9	Pass					
LHS taper, far/near (%)			52.7	Pass					
RHS taper, far/near (%)			51.9	Pass					
Pos (mm)	LHS centr (bins)	LHS rms (bins)	LHS FWHM (%)	RHS centr (bins)	RHS rms (bins)	RHS FWHM (%)	Avg centr (bins)	Avg rms (bins)	Avg FWHM (%)
020	428.1	30.5	16.7	242.8	20.6	19.9	331.0	18.4	13.0
050	396.5	30.2	17.9	258.3	20.9	19.0	328.3	18.2	13.0
080	365.9	29.8	19.1	279.4	21.1	17.7	332.3	17.8	12.6
…	…	…	…	…	…	…	…	…	…
320	232.5	20.7	20.9	435.9	31.8	17.1	332.0	18.3	13.0
350	225.4	20.1	21.0	468.1	31.1	15.6	341.3	18.1	12.5

6.7.5 Fit summary table

The analysis software shall produce an ASCII summary table of the best-fit parameters measured at each end and the average for each test position. Each row of the table shall correspond to a single test position, and it shall contain 19 columns, corresponding to the scan position (in mm), the six parameters of the LHS fit in the order given in Section 6.4, the six parameters of the RHS fit, and the six parameters of the fit to the average spectrum. This table shall be logged to a file with filename `Crystal ID + Version + '.xls'`.